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Energy-Based Probabilistic Regression in Computer Vision

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Uppsala University

Half-time seminar
February 3, 2022

[Paper I] Energy-Based Models for Deep Probabilistic Regression
Fredrik K. Gustafsson, Martin Danelljan, Goutam Bhat, Thomas B. Schön
The European Conference on Computer Vision (ECCV), 2020

[Paper II] How to Train Your Energy-Based Model for Regression
Fredrik K. Gustafsson, Martin Danelljan, Radu Timofte, Thomas B. Schön
The British Machine Vision Conference (BMVC), 2020

[Paper III] Accurate 3D Object Detection using Energy-Based Models
Fredrik K. Gustafsson, Martin Danelljan, Thomas B. Schön
The IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR) Workshops, 2021

[Paper IV] Learning Proposals for Practical Energy-Based Regression
Fredrik K. Gustafsson, Martin Danelljan, Thomas B. Schön
The International Conference on Artificial Intelligence and Statistics (AISTATS), 2022

Outline

Energy-based models.

Energy-based models for regression.

How to train energy-based models for regression.

- Noise contrastive estimation (NCE).

Energy-based regression for 3D object detection.

Practical limitations of energy-based regression.

Learning proposals for more practical energy-based regression.

Energy-Based Models

Energy-based models have a rich history within machine learning.

An **energy-based model (EBM)** specifies a probability distribution $p(x;\theta)$ over $x \in \mathcal{X}$ directly via a parameterized scalar function $f_\theta : \mathcal{X} \to \mathbb{R}$:

$$p(x;\theta) = \frac{e^{f_\theta(x)}}{Z(\theta)}, \quad Z(\theta) = \int e^{f_\theta(\tilde{x})} d\tilde{x}$$

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EBMs have therefore become increasingly popular within computer vision in recent years, commonly being applied for various generative image modeling tasks.

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Compare with normalizing flow models which are specifically designed to be easy to both evaluate and sample. EBMs instead prioritize maximum model expressivity.

While EBMs recently had become increasingly popular within computer vision, they were basically only being employed for generative image modeling.

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In **[Paper I] Energy-Based Models for Deep Probabilistic Regression**, we instead explored the application of EBMs to various regression problems.

Regression: learn to predict a continuous target $y^\star \in \mathcal{Y} = \mathbb{R}^K$ from a corresponding input $x^\star \in \mathcal{X}$, given a training set $\mathcal{D}$ of i.i.d. input-target pairs, $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$, $(x_i, y_i) \sim p(x, y)$.

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We employ a probabilistic regression approach, using a *conditional* EBM to model the predictive distribution $p(y|x)$ of the regression target y given the input x:

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Here, $f_\theta : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ is a DNN that maps any input-target pair $(x, y) \in \mathcal{X} \times \mathcal{Y}$ directly to a scalar $f_\theta(x, y) \in \mathbb{R}$, and $Z(x, \theta)$ is the input-dependent partition function.

Energy-Based Probabilistic Regression

Energy-Based Probabilistic Regression: train a DNN $f_\theta : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$ to predict a scalar $f_\theta(x, y)$, then model $p(y|x)$ with the conditional EBM $p(y|x;\theta)$:

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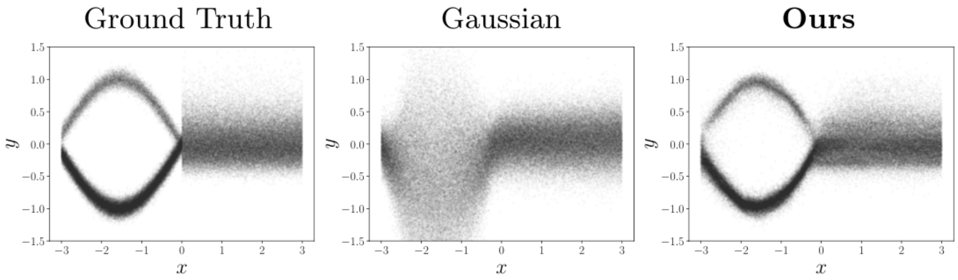
The EBM $p(y|x;\theta)$ can learn complex distributions $p(y|x)$ directly from data:



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Paper I:

- Age estimation, $\mathcal{Y} = \mathbb{R}$.
- Head-pose estimation, $\mathcal{Y} = \mathbb{R}^3$.
- 2D bounding box regression (object detection, visual tracking), $\mathcal{Y} = \mathbb{R}^4$.

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- 3D bounding box regression (3D object detection in LiDAR point clouds), $\mathcal{Y} = \mathbb{R}^7$.

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Paper IV:

- Steering angle prediction, $\mathcal{Y} = \mathbb{R}$.
- Cell-count prediction, $\mathcal{Y} = \mathbb{R}$.
- Age estimation, $\mathcal{Y} = \mathbb{R}$.
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In **Paper I, II & III**, we predict the most likely target under the model given an input $x^\star$ at test-time, i.e. $y^\star = \text{argmax}_y\, p(y|x^\star;\theta) = \text{argmax}_y\, f_\theta(x^\star, y)$.

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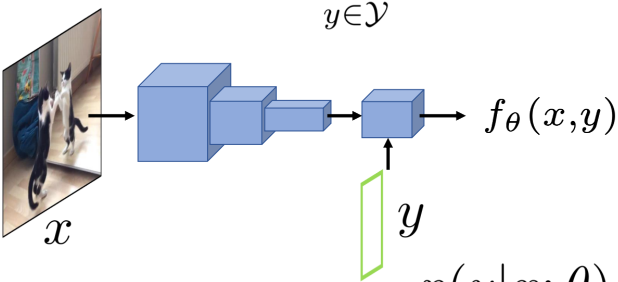
In practice, $y^\star = \text{argmax}_y \, f_\theta(x^\star, y)$ is approximated by refining an initial estimate $\hat{y}$ via T steps of gradient ascent,

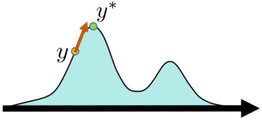
$$y \leftarrow y + \lambda \nabla_y f_\theta(x^\star, y),$$

thus finding a local maximum of $f_\theta(x^\star, y)$. Evaluation of the partition function $Z(x^\star, \theta)$ is therefore *not* required.

Energy-Based Probabilistic Regression - Prediction

$$y^* = \underset{y \in \mathcal{Y}}{\arg\max}\, p(y|x;\theta) = \underset{y \in \mathcal{Y}}{\arg\max}\, f_\theta(x,y)$$





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The DNN $f_\theta(x, y)$ can be trained using various methods for fitting a distribution $p(y|x;\theta)$ to observed data $\{(x_i, y_i)\}_{i=1}^N$.

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In general, the most straightforward such method is probably to minimize the negative log-likelihood $\mathcal{L}(\theta) = -\sum_{i=1}^N \log p(y_i|x_i;\theta)$, which for the EBM $p(y|x;\theta)$ is given by,

$$\mathcal{L}(\theta) = \sum_{i=1}^N \log\Big(\int e^{f_\theta(x_i,y)} dy\Big) - f_\theta(x_i, y_i).$$

Energy-Based Probabilistic Regression - Training

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In **[Paper I] Energy-Based Models for Deep Probabilistic Regression**, we simply approximated this intractable integral using importance sampling.

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Importance sampling:

$$\begin{aligned}
-\log p(y_i|x_i;\theta) &= \log\left(\int e^{f_\theta(x_i,y)} dy\right) - f_\theta(x_i, y_i) \\
&= \log\left(\int \frac{e^{f_\theta(x_i,y)}}{q(y)} q(y) dy\right) - f_\theta(x_i, y_i) \\
&\approx \log\left(\frac{1}{M}\sum_{m=1}^{M} \frac{e^{f_\theta(x_i,y^{(m)})}}{q(y^{(m)})}\right) - f_\theta(x_i, y_i), \quad y^{(m)} \sim q(y).
\end{aligned}$$

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Various alternative techniques could however also be employed to train the DNN $f_\theta(x, y)$, including noise contrastive estimation (NCE), score matching and MCMC.

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We compared six methods on the task of 2D bounding box regression, and concluded that a simple extension of NCE should be considered the go-to training method.

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Specifically, the DNN $f_\theta(x,y)$ is trained by minimizing $J_{\text{NCE}}(\theta) = -\frac{1}{N}\sum_{i=1}^{N} J_{\text{NCE}}^{(i)}(\theta)$,

$$J_{\text{NCE}}^{(i)}(\theta) = \log \frac{\exp\{f_\theta(x_i, y_i^{(0)}) - \log q(y_i^{(0)})\}}{\sum_{m=0}^{M} \exp\{f_\theta(x_i, y_i^{(m)}) - \log q(y_i^{(m)})\}},$$

where $y_i^{(0)} \triangleq y_i$, and $\{y_i^{(m)}\}_{m=1}^{M}$ are M samples drawn from a noise distribution $q(y)$.

Energy-Based Probabilistic Regression - Training using NCE

$$J_{\mathrm{NCE}}(\theta) = -\frac{1}{N}\sum_{i=1}^{N} J_{\mathrm{NCE}}^{(i)}(\theta), \quad J_{\mathrm{NCE}}^{(i)}(\theta) = \log \frac{\exp\{f_\theta(x_i, y_i^{(0)}) - \log q(y_i^{(0)})\}}{\sum_{m=0}^{M} \exp\{f_\theta(x_i, y_i^{(m)}) - \log q(y_i^{(m)})\}},$$

$$y_i^{(0)} \triangleq y_i, \quad \{y_i^{(m)}\}_{m=1}^{M} \sim q(y) \text{ (noise distribution)}.$$

Energy-Based Probabilistic Regression - Training using NCE

$$J_{\mathrm{NCE}}(\theta) = -\frac{1}{N}\sum_{i=1}^{N} J_{\mathrm{NCE}}^{(i)}(\theta), \quad J_{\mathrm{NCE}}^{(i)}(\theta) = \log \frac{\exp\{f_\theta(x_i, y_i^{(0)}) - \log q(y_i^{(0)})\}}{\sum_{m=0}^{M} \exp\{f_\theta(x_i, y_i^{(m)}) - \log q(y_i^{(m)})\}},$$

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Effectively, $J_{\mathrm{NCE}}(\theta)$ is the softmax cross-entropy loss for a classification problem with $M+1$ classes (which of the $M+1$ values $\{y_i^{(m)}\}_{m=0}^{M}$ is the true target y_i?).

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In **[Paper II] How to Train Your Energy-Based Model for Regression**, the noise distribution $q(y)$ was set to a mixture of K Gaussians centered at the true target y_i,

$$q(y) = \frac{1}{K}\sum_{k=1}^{K} \mathcal{N}(y; y_i, \sigma_k^2 I).$$

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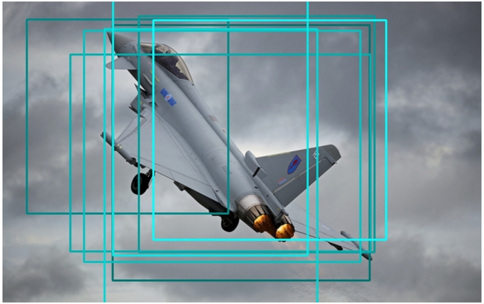

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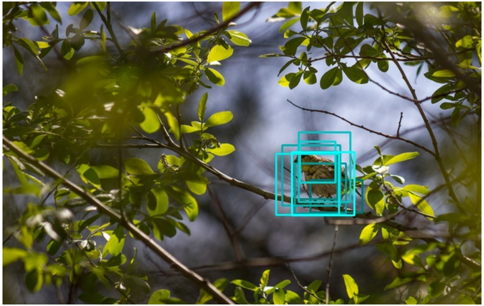
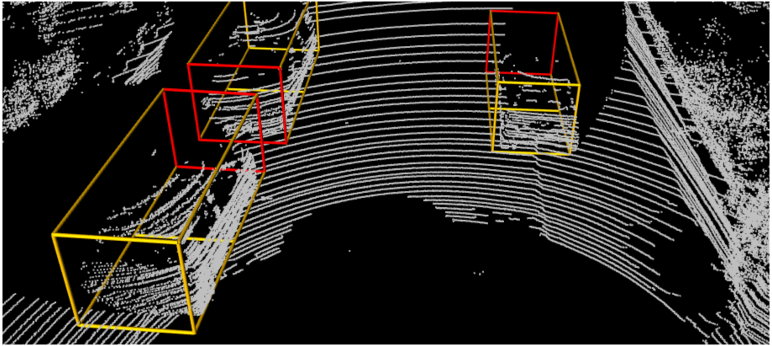


Energy-Based Probabilistic Regression - 3D Object Detection



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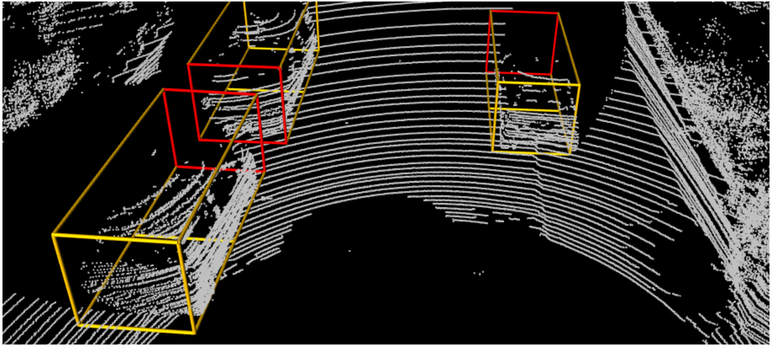
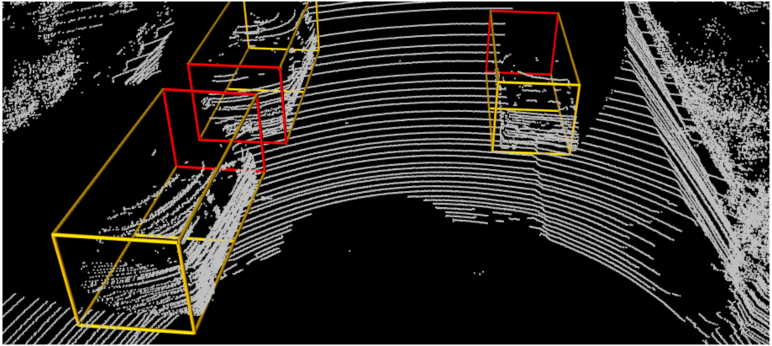


In **[Paper III] Accurate 3D Object Detection using Energy-Based Models**, we extend our energy-based regression approach from 2D to 3D bounding box regression.

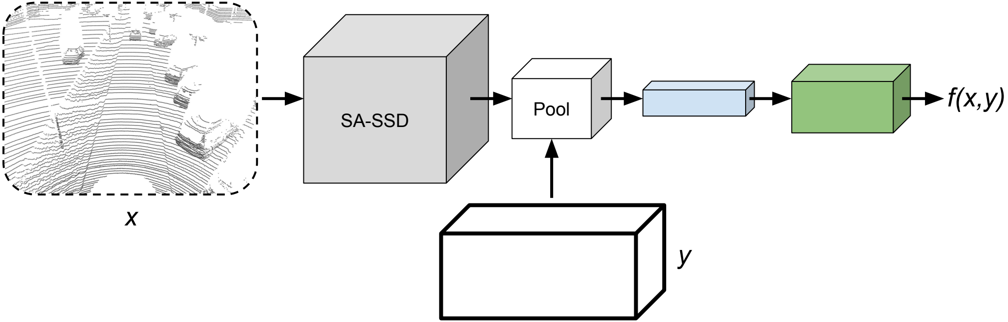
Energy-Based Probabilistic Regression - 3D Object Detection

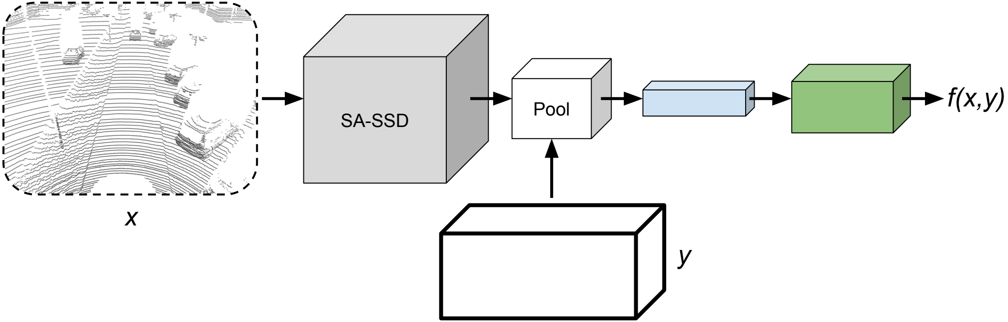


In **[Paper III] Accurate 3D Object Detection using Energy-Based Models**, we extend our energy-based regression approach from 2D to 3D bounding box regression.

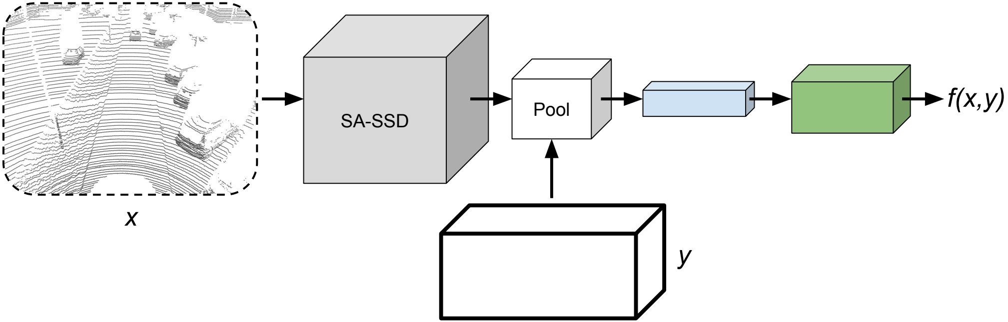
This is achieved by designing a differentiable pooling operator for 3D bounding boxes $y \in \mathbb{R}^7$, and adding an extra network branch to a state-of-the-art 3D object detector.

Energy-Based Probabilistic Regression - 3D Object Detection





We integrate a conditional EBM $p(y|x;\theta) = e^{f_\theta(x,y)} / \int e^{f_\theta(x,\tilde{y})} d\tilde{y}$ into the SA-SSD 3D object detector.



We integrate a conditional EBM $p(y|x;\theta) = e^{f_\theta(x,y)} / \int e^{f_\theta(x,\tilde{y})} d\tilde{y}$ into the SA-SSD 3D object detector.

We design a differentiable pooling operator that, given a 3D bounding box y, extracts a feature vector from the SA-SSD output. This feature vector is processed by fully-connected layers, outputting $f_\theta(x, y) \in \mathbb{R}$.

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In **Paper I**, we trained the EBM $p(y|x;\theta)$ by approximating the negative log-likelihood $\mathcal{L}(\theta) = -\sum_{i=1}^{N} \log p(y_i|x_i;\theta)$ using importance sampling:

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N} \log\left(\frac{1}{M}\sum_{m=1}^{M} \frac{e^{f_\theta(x_i, y_i^{(m)})}}{q(y_i^{(m)})}\right) - f_\theta(x_i, y_i),$$

$$\{y_i^{(m)}\}_{m=1}^{M} \sim q(y) \text{ (proposal distribution).}$$

Energy-Based Probabilistic Regression - Practical Limitations

In **Paper II & III**, we trained the EBM $p(y|x;\theta)$ using NCE:

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$$y_i^{(0)} \triangleq y_i, \quad \{y_i^{(m)}\}_{m=1}^{M} \sim q(y) \text{ (noise distribution).}$$

In both cases, the proposal/noise distribution $q(y)$ was set to a mixture of K Gaussian components centered at the true target y_i,

$$q(y) = \frac{1}{K}\sum_{k=1}^{K} \mathcal{N}(y; y_i, \sigma_k^2 I).$$

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The proposal/noise distribution $q(y)$ depends on the true target y_i, and can therefore only be utilized during training.

- To produce a prediction $y^\star$ at test-time, **Paper I, II & III** employed gradient ascent to refine an initial estimate $\hat{y}$. However, this prediction strategy then requires access to good initial estimates.

Energy-Based Probabilistic Regression - Practical Limitations

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In **[Paper IV] Learning Proposals for Practical Energy-Based Regression**, we address both these limitations by jointly learning a parameterized proposal/noise distribution $q(y|x;\phi)$ during EBM training.

We derive an efficient and convenient objective that can be employed to train $q(y|x;\phi)$ by directly minimizing its KL divergence to the EBM $p(y|x;\theta)$.

We want $q(y|x;\phi)$ to be a close approximation of the EBM $p(y|x;\theta)$. Specifically, we want to find ϕ that minimizes the KL divergence between $q(y|x;\phi)$ and $p(y|x;\theta)$.

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Therefore, we seek to compute $\nabla_\phi D_{\mathrm{KL}}\big(p(y|x;\theta) \parallel q(y|x;\phi)\big)$. The gradient $\nabla_\phi D_{\mathrm{KL}}$ is generally intractable, but can be conveniently approximated by the following result:

Practical Energy-Based Regression - Learning the Proposal

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Result 1: For a conditional EBM $p(y|x;\theta) = e^{f_\theta(x,y)} / \int e^{f_\theta(x,\tilde{y})} d\tilde{y}$ and distribution $q(y|x;\phi)$,

$$\nabla_\phi D_{\mathrm{KL}}\big(p \parallel q\big) \approx \nabla_\phi \log\left(\frac{1}{M}\sum_{m=1}^{M} \frac{e^{f_\theta(x,y^{(m)})}}{q(y^{(m)}|x;\phi)}\right),$$

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Given data $\{x_i\}_{i=1}^{N}$, Result 1 implies that the proposal/noise distribution $q(y|x;\phi)$ can be trained to approximate the EBM $p(y|x;\theta)$ by minimizing the loss,

$$J_{\mathrm{KL}}(\phi) = \frac{1}{N}\sum_{i=1}^{N} \log\left(\frac{1}{M}\sum_{m=1}^{M} \frac{e^{f_\theta(x_i,y_i^{(m)})}}{q(y_i^{(m)}|x_i;\phi)}\right),$$

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Practical Energy-Based Regression - Joint Training Method

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$J(\theta)$ can thus be used as a joint objective for training both q and the EBM p.

Practical Energy-Based Regression - Joint Training Method

$$J(\theta, \phi) = \frac{1}{N} \sum_{i=1}^{N} \log \left(\frac{1}{M} \sum_{m=1}^{M} \frac{e^{f_\theta(x_i, y_i^{(m)})}}{q(y_i^{(m)}|x_i; \phi)} \right) - f_\theta(x_i, y_i),$$

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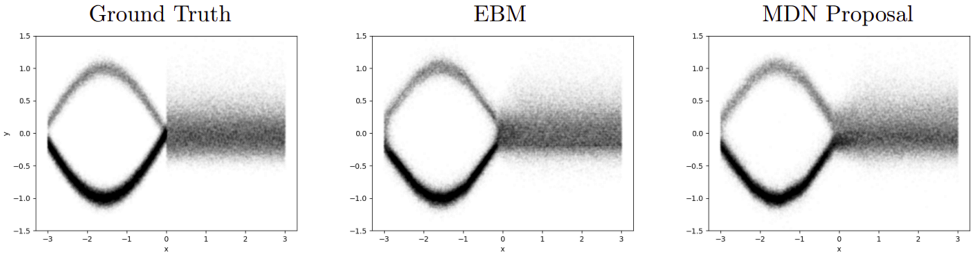
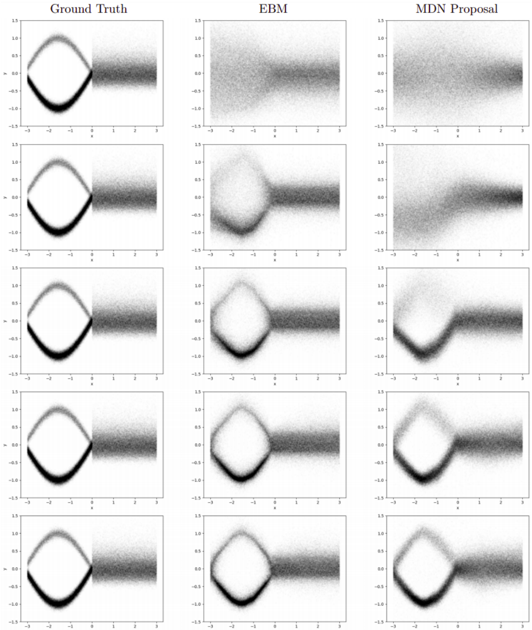
$$\{y_i^{(m)}\}_{m=1}^{M} \sim q(y|x_i; \phi).$$

The EBM $p(y|x;\theta)$ and proposal $q(y|x;\phi)$ can be trained by jointly minimizing $J(\theta,\phi)$ w.r.t. both θ and ϕ:



Practical Energy-Based Regression - Joint Training Method



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The EBM $p(y|x;\theta)$ and proposal/noise distribution $q(y|x;\phi)$ can also be jointly trained by updating ϕ via the loss $J_{\mathrm{KL}}(\phi)$, and updating θ via $J_{\mathrm{NCE}}(\theta)$.

Practical Energy-Based Regression - Utilizing the Proposal

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We have access to a proposal $q(y|x;\phi)$ that is conditioned only on the input x and thus can be utilized also at test-time.

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As $q(y|x;\phi)$ has been trained to approximate the EBM $p(y|x;\theta)$, it can be utilized with self-normalized importance sampling to approximate expectations $\mathbb{E}_p$ w.r.t. the EBM,

$$\mathbb{E}_p[\xi(y)] = \int \xi(y) p(y|x;\theta) dy \approx \sum_{m=1}^{M} w^{(m)} \xi\big(y^{(m)}\big),$$

$$w^{(m)} = \frac{e^{f_\theta(x, y^{(m)})} / q(y^{(m)}|x;\phi)}{\sum_{l=1}^{M} e^{f_\theta(x, y^{(l)})} / q(y^{(l)}|x;\phi)},$$

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where $\{y^{(m)}\}_{m=1}^{M} \sim q(y|x;\phi)$.

Setting $\xi(y) = y$ enables us to approximately compute the EBM mean. In this manner, we can thus directly produce a stand-alone prediction $y^\star$ for the EBM $p(y|x;\theta)$.

Practical Energy-Based Regression - Utilizing the Proposal

$$w^{(m)} = \frac{e^{f_\theta(x, y^{(m)})}/q(y^{(m)}|x;\phi)}{\sum_{l=1}^{M} e^{f_\theta(x, y^{(l)})}/q(y^{(l)}|x;\phi)}$$

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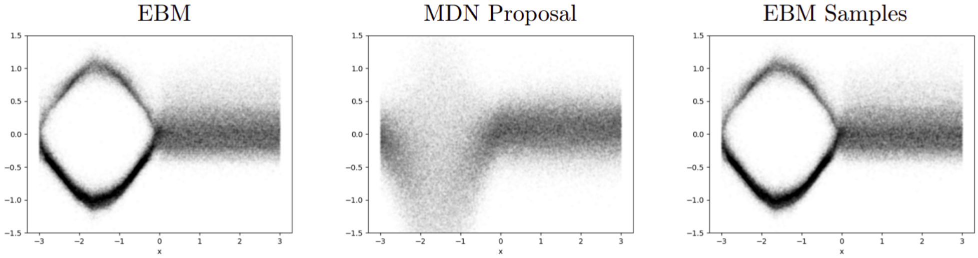
We can also draw approximate samples from the EBM $p(y|x; \theta)$ by re-sampling with replacement from the set $\{y^{(m)}\}_{m=1}^{M} \sim q(y|x; \phi)$ of proposal samples, drawing each $y^{(m)}$ with probability $w^{(m)}$:



Summary

Energy-based models.

Energy-based models for regression.

How to train energy-based models for regression.

- Noise contrastive estimation (NCE).

Energy-based regression for 3D object detection.

Practical limitations of energy-based regression.

Learning proposals for more practical energy-based regression.

Contact

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